High-Fidelity Numerical Modeling of Spray Droplet Formation
2023 IFPRI Annual General Meeting

Olivier Desjardins and Joseph Giliberto
Sibley School of Mechanical and Aerospace Engineering, Cornell University

Motivation

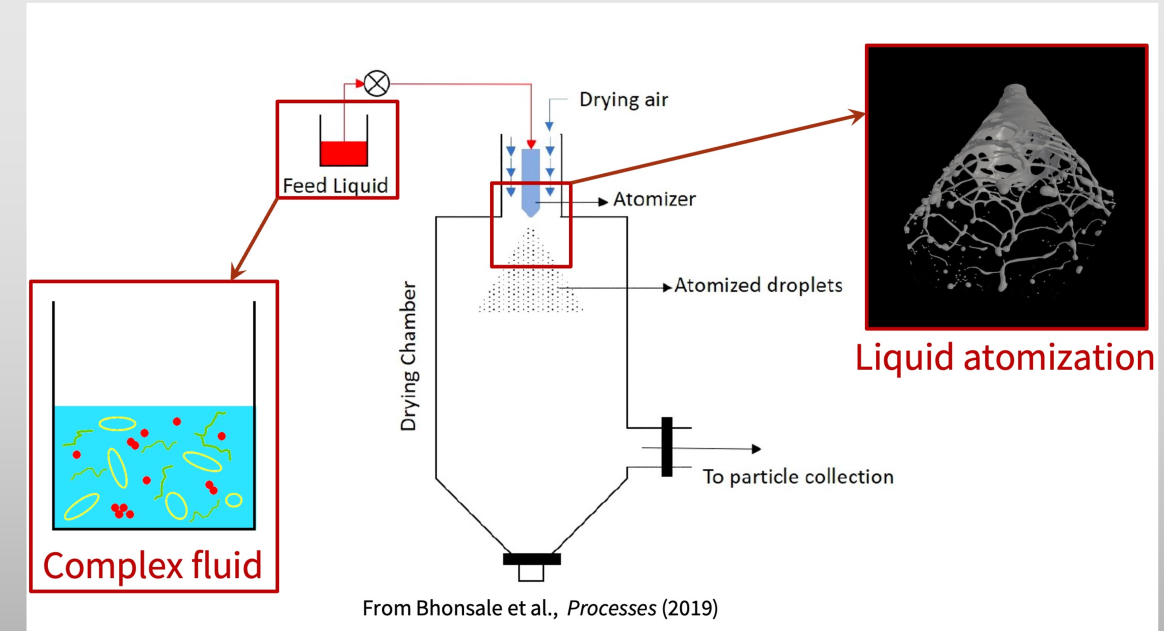
- Many industrial processes such as spray drying for powder production rely on **atomizing complex fluids** into a spray
- **Complex liquid rheology adds significant challenges** to a phenomenon that is already challenging to model and predict

Objective

- Assess and enhance ability of our novel high-fidelity multiscale spray atomization model for complex fluids

Accomplishments

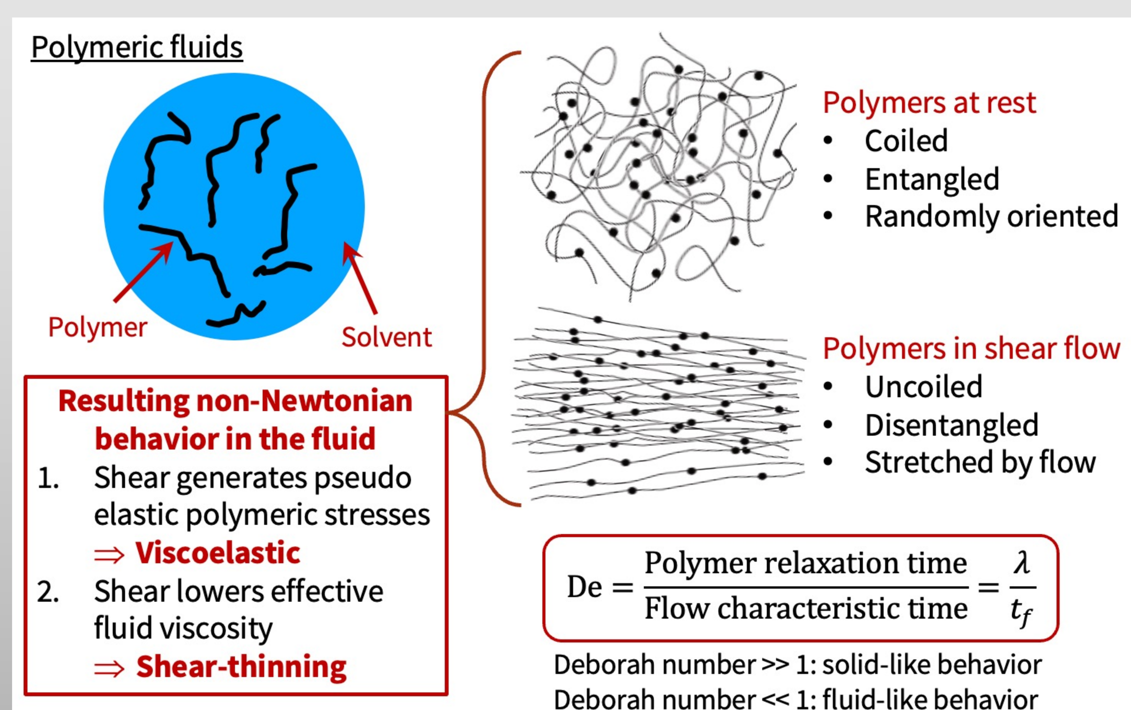
- Assess influence of high viscosity fluid in pressure swirl configuration
- Identify experimental datasets for complex fluid atomization
- Implemented non-Newtonian model in flow solver



From Bhonsale et al., *Processes* (2019)

Complex fluid phenomena

- High effective viscosity, shear-rate-dependent viscosity, viscoelasticity, viscoplasticity, etc…



Mathematical model

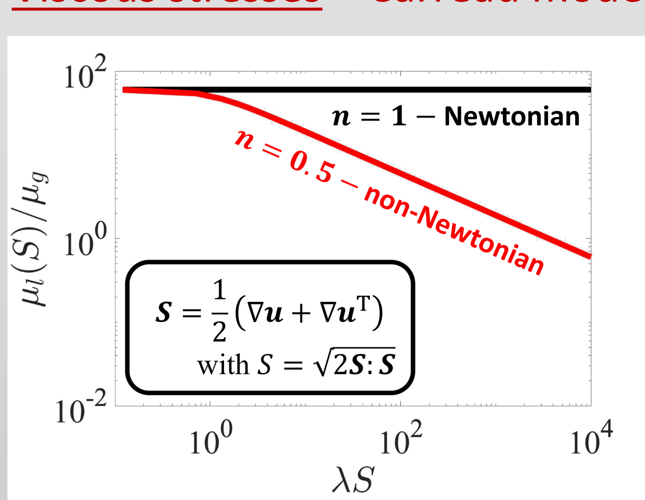
Continuity: $\nabla \cdot \boldsymbol{u} = 0$

Liquid volume conservation: $\frac{\partial \alpha}{\partial t} + \boldsymbol{u} \cdot \nabla \alpha = 0$

Momentum conservation:

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \nabla \cdot \boldsymbol{\tau}_p + \nabla \cdot \boldsymbol{\tau}_{sgs} + \boldsymbol{F}_{ST}$$

Viscous stresses – Carreau model



$$\boldsymbol{\tau} = 2\mu \boldsymbol{S}$$

$$\rho = \alpha \rho_l + (1-\alpha)\rho_g$$

$$\mu = \alpha \mu_l + (1-\alpha)\mu_g$$

$\mu_l = \mu_s + \mu_p$ with

$$\mu_p = \mu_{p,0}\left(1 + (\lambda S)^2\right)^{\frac{n-1}{2}}$$

Elastic stresses – FENE-CR model

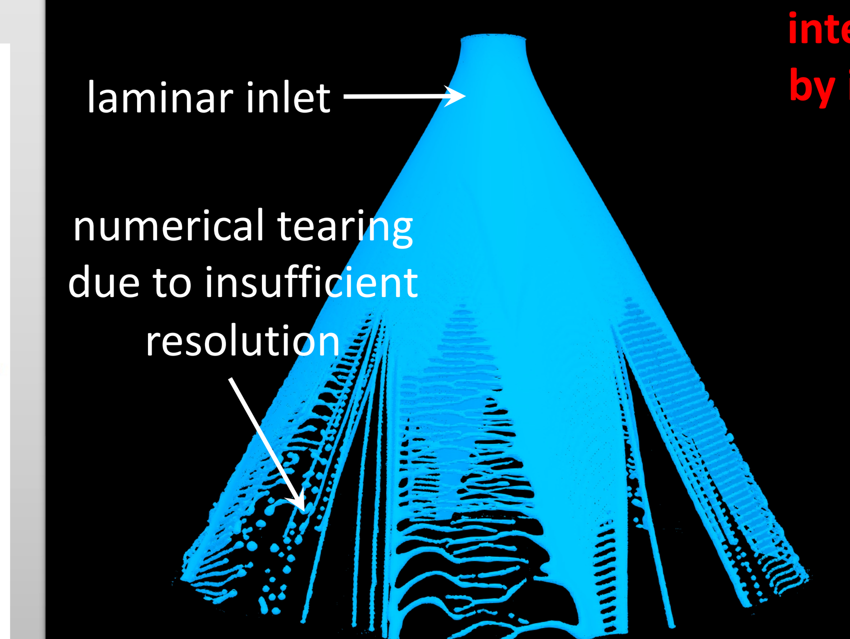
$$\boldsymbol{\tau}_p = \mu_p f \frac{\mathbf{C} - \mathbf{I}}{\lambda}$$

- Elastic dumbbells model of polymers
- Represents a Boger fluid
- $\mathbf{C}$ = conformation tensor and $\mathbf{I}$ = identity tensor
- and $\mathbf{C}$ is solution of

$$\frac{\partial \mathbf{C}}{\partial t} + \boldsymbol{u} \cdot \nabla \mathbf{C} = \nabla \boldsymbol{u} \cdot \mathbf{C} + \mathbf{C} \cdot (\nabla \boldsymbol{u})^T - f\frac{\mathbf{C} - \mathbf{I}}{\lambda}$$

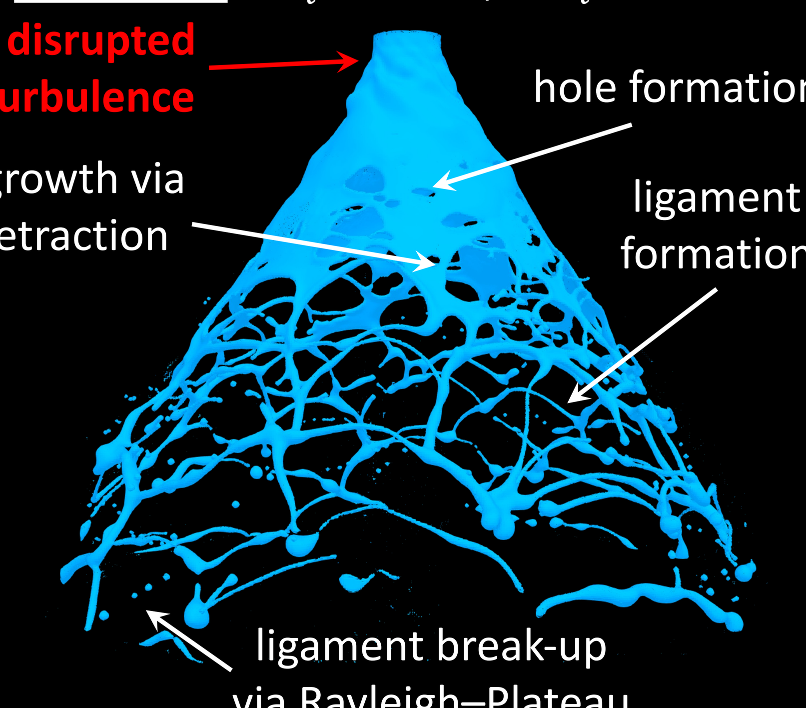
Pressure-swirl atomization

Newtonian: $\mathrm{Re}_l = 100$, $\mathrm{We}_l = 1000$



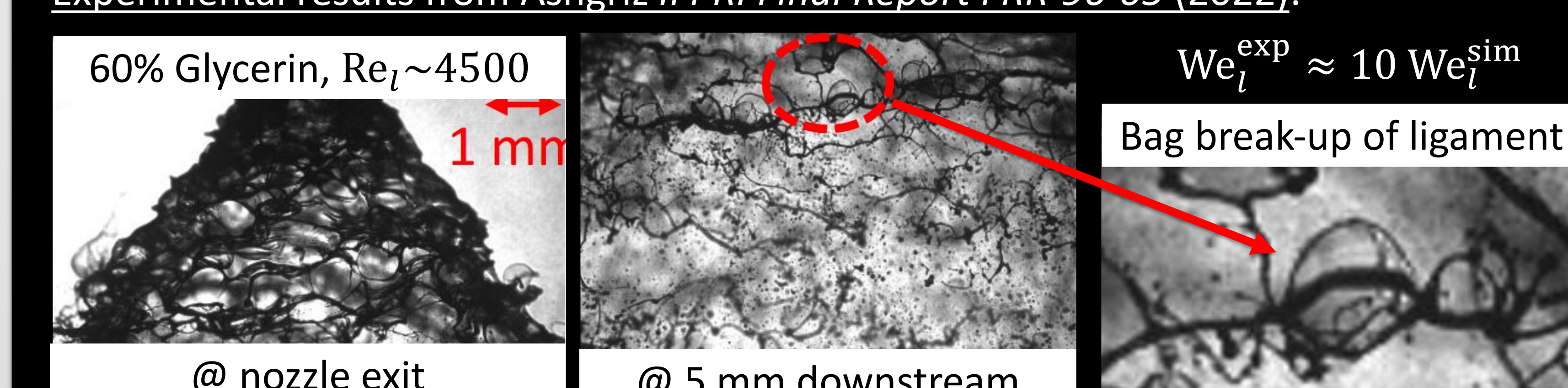
No atomization in domain

Newtonian: $\mathrm{Re}_l = 5000$, $\mathrm{We}_l = 1000$

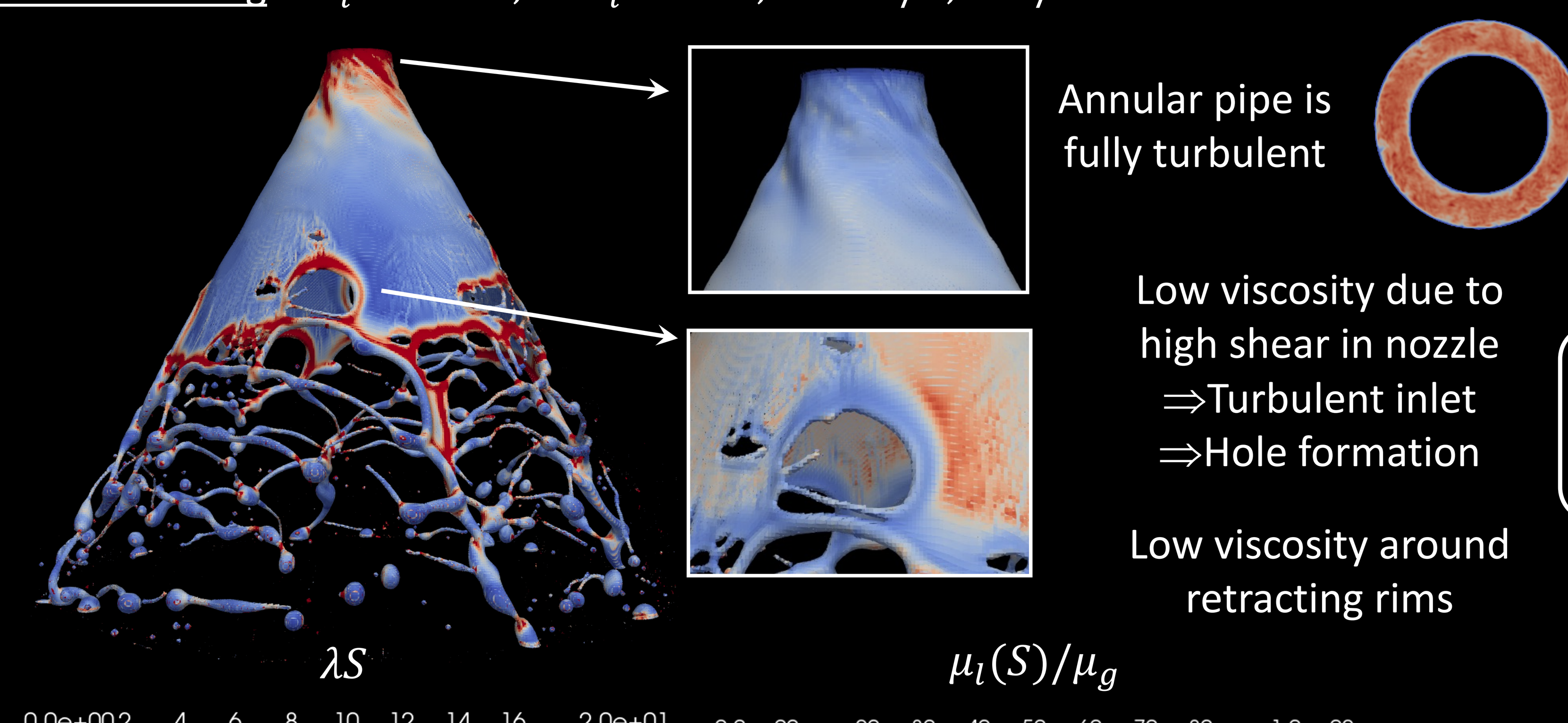


Atomization partially captured in domain

Experimental results from Ashgriz *IFPRI Final Report FRR-96-05* (2022):



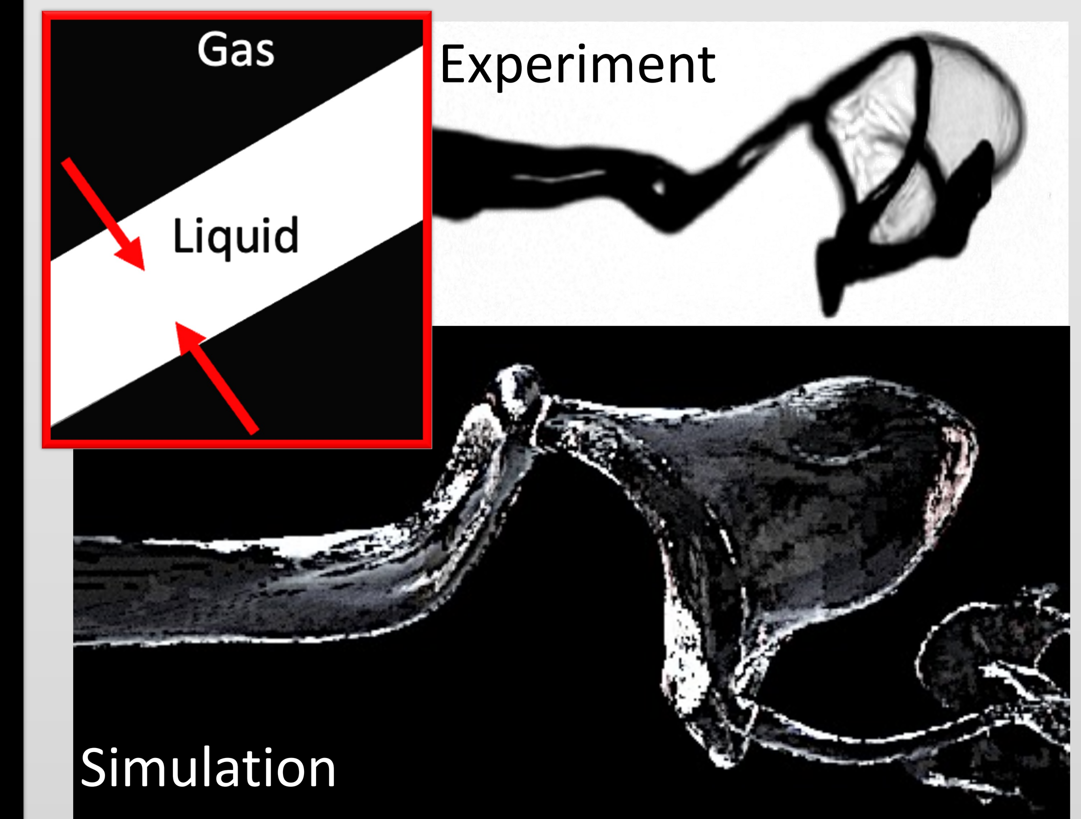
Shear-thinning: $\mathrm{Re}_l = 1000$, $\mathrm{We}_l = 500$, $n = 1/2$, $\lambda D/U = 10$



Ongoing model development

Sub-grid tracking of interfacial structures

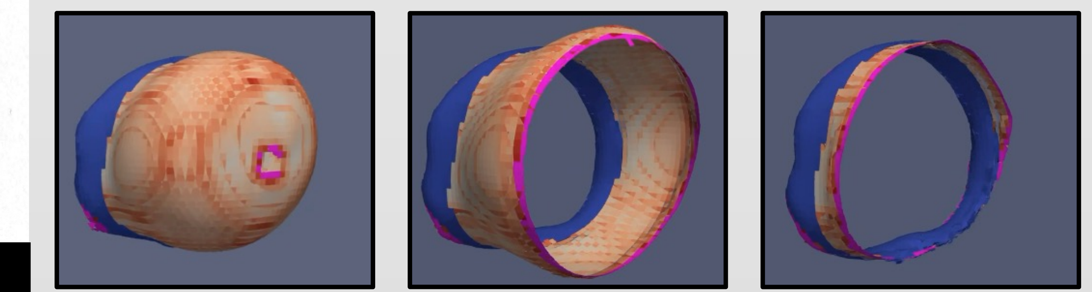
- Interface reconstruction with two planes in each cell maintains sub-grid-thickness films



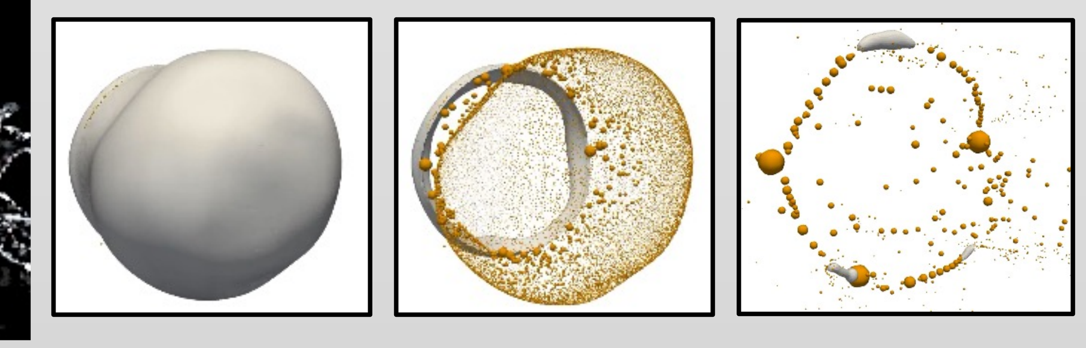
Sub-grid scale breakup modeling

- Films are detected and are treated with two possible models

1. Undergo Taylor-Culick retraction

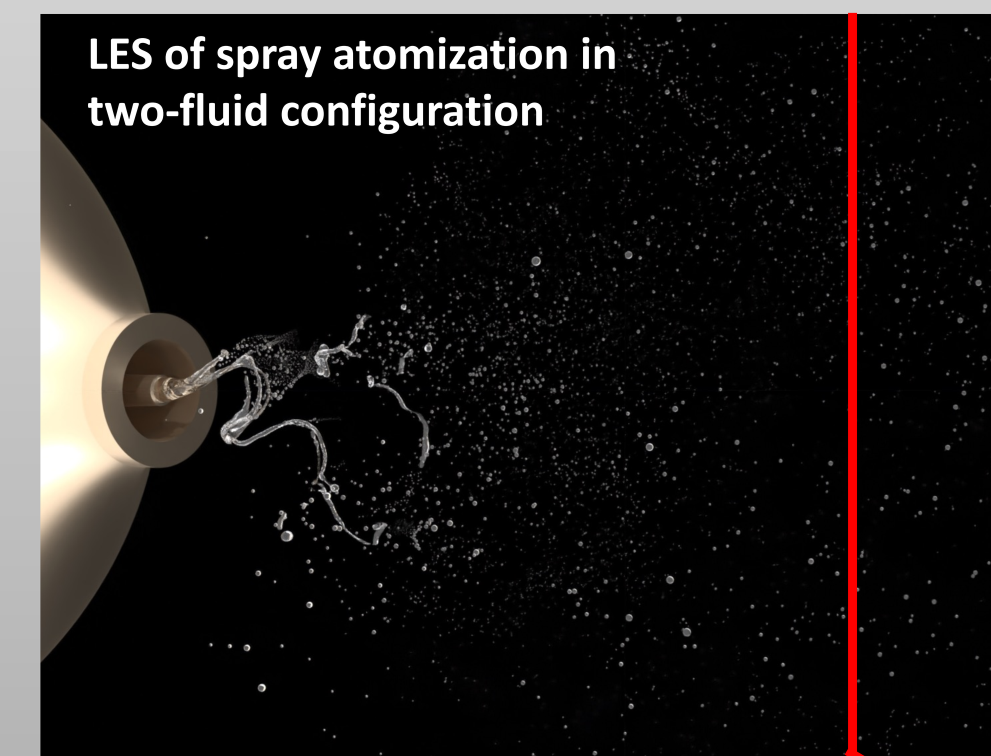


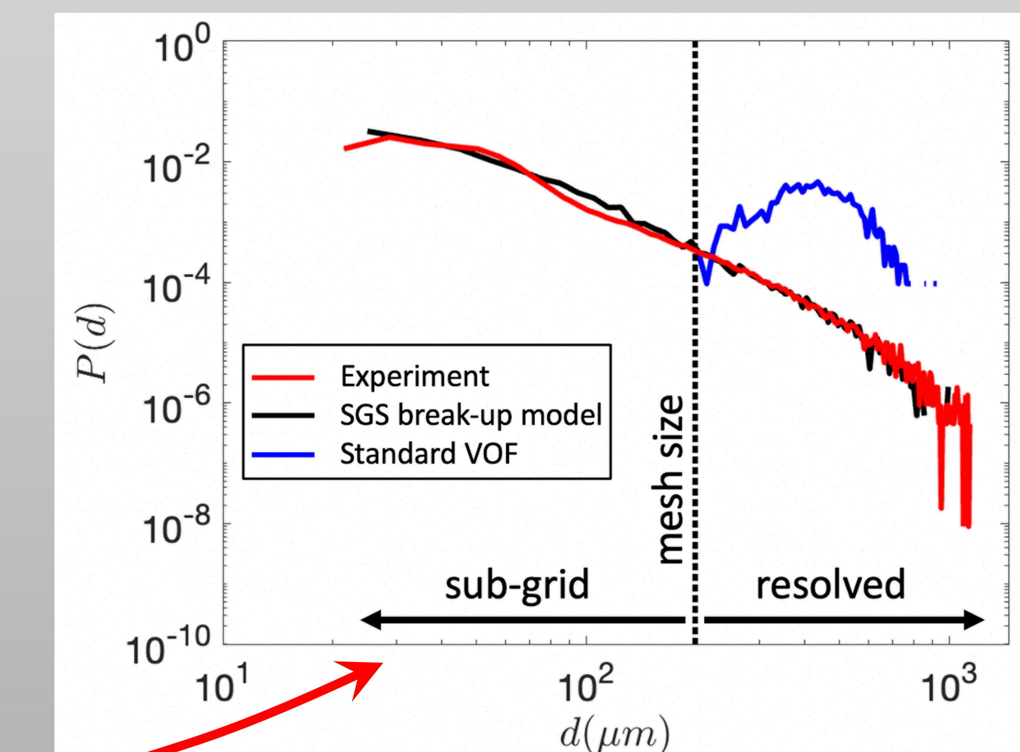
2. Undergo instantaneous bursting



High-fidelity multiscale modeling of atomization

- Recently developed multiscale modeling framework for spray atomization shows promise for mesh-independent drop size predictions





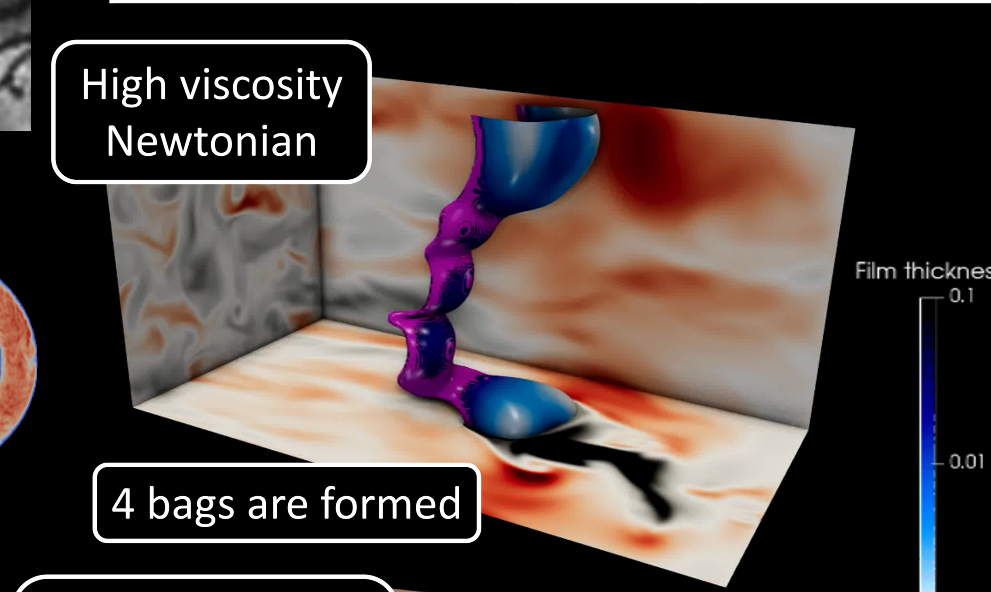
Isolated ligament break-up in a cross-flow

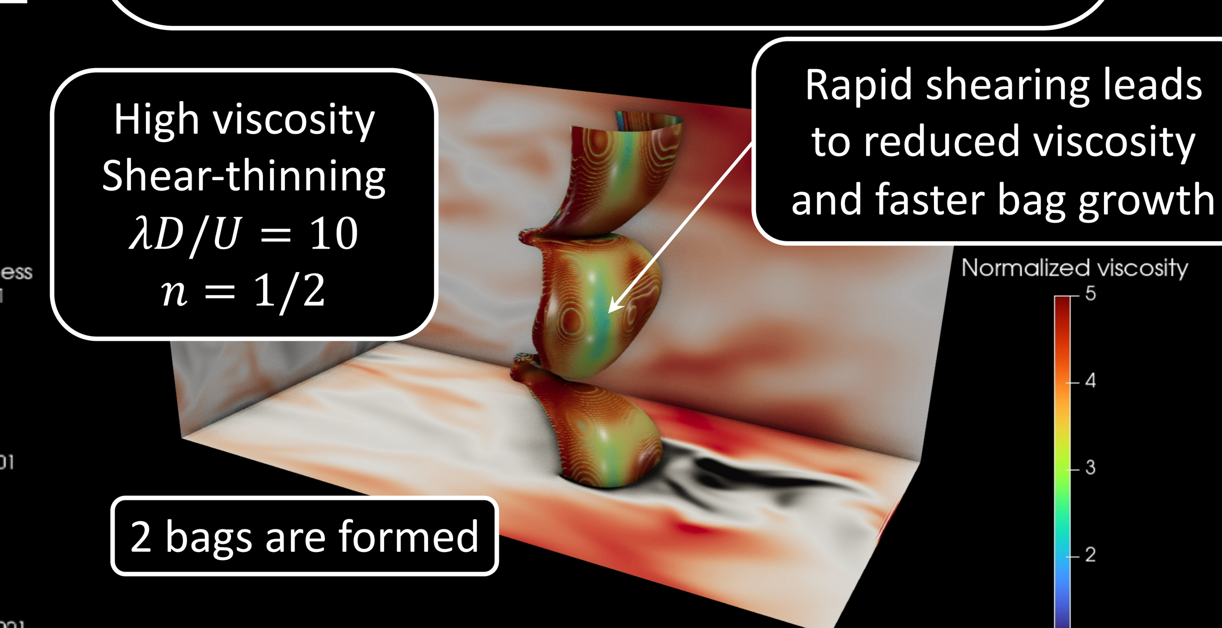
Model	μ_l/μ_g	ρ_l/ρ_g
Newtonian	50	1000
Newtonian	500	1000
Shear-thinning	500	1000
Shear-thinning and viscoelastic	500	1000

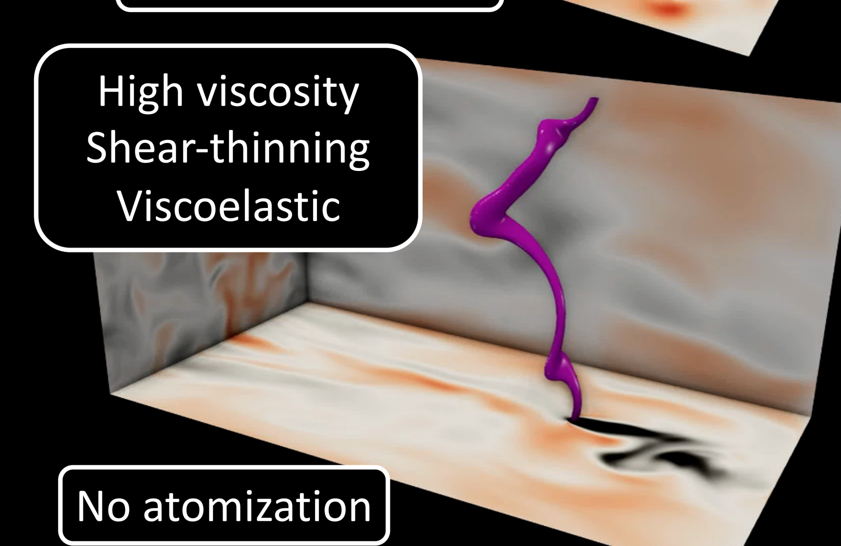
- Liquid ligament is accelerated by gas ⇒Susceptible to **Rayleigh–Taylor instability**
- Most unstable wavelength given by

$$\frac{\lambda_{RT}}{D} = \sqrt{\frac{6\pi^3 \rho_l}{C_D(\rho_l - \rho_g)}}\,\mathrm{We}_g^{-\frac{1}{2}}$$

- Inviscid theory predicts 6 bags in simulation







Future steps

- Further validation of complex, viscoelastic fluid models
- Quantitative comparison examining the impact of high viscosity and complex rheology:
  - Pressure swirl atomization
  - Isolated ligament in turbulent cross flow